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TECHNICAL REPORT BRL-TR-2622

AN ADVANCED FLASH SUPPRESSION  
NETWORK INVOLVING ALKALI SALTS

Joseph M. Heimerl

December 1984

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The kinetic network to be described in this report was deduced by a systematic and duplicable methodology.

The reactive species are: H, O, OH, H<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>O, and HO<sub>2</sub>; together with CO and CO<sub>2</sub>; and the suppression species: K, KO, KO<sub>2</sub>, KOH, and KH. (N<sub>2</sub> is a nonreactive diluent.) All unimolecular, two- and three-body reactions possible among this set of reactive species were generated. Reactions in which multiple bonds were broken were eliminated from further consideration. Where possible, rate coefficients for the remaining reactions were taken from the literature. Those for which no literature values could be found were assigned gas-kinetic values.

This network, consisting of 48 reactions, was used in the MEFF muzzle-flash-prediction code for M30 propellant with 1% and 2.7% K<sub>2</sub>SO<sub>4</sub> added. The code results agree with previous MEFF calculations and with the observations that flash is observed in the former and not the latter case.

To further eliminate unimportant reactions, the hydrogen/air/suppressant network was employed in a flat flame model. By analysis of four different fuel/air ratio mixtures, many other reactions were eliminated. In addition, this analysis indicated the reactions which dominate and the reactions for which rate coefficients need to be measured.

This abbreviated network, consisting of 32 reactions, was again employed in MEFF calculations with results nearly identical to those above.

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## I. INTRODUCTION

This paper is a sequel to an earlier work on muzzle flash and its suppression from an elementary kinetic point of view.<sup>1</sup> In the earlier report we discussed definitions of terms, the importance of the problem, the options available to suppress the flash, and several apparently contradictory laboratory results on flame inhibition. The present paper builds upon the recent work of Hynes, Steinberg, and Schofield<sup>2</sup> to produce a hypothetical but realistic suppression network of elementary chemical reactions. The most important aspect of the present work is the methodology employed to construct the network. The methodology is quite general and can be used iteratively as more accurate data (species or rate coefficients) become known.

We shall begin with a brief review of the problem (see Reference 1 for more details), then illustrate the methodology by actually constructing a suppression network.

The effluent from a large artillery piece is known to consist of a fuel rich mixture containing  $H_2$  and CO. Upon mixing with the surrounding air, a combustion process can take place that results in a high intensity flash. This phenomenon is called secondary muzzle flash or simply muzzle flash. About one half the energy of the propellant can be found in this effluent, so that muzzle flash can be accompanied by a substantial blast. In the past both this flash and blast have been suppressed in many weapons by the addition of alkali salts, usually potassium sulfate or potassium nitrate. Since only a few percent (by weight) salt addition has been found to be effective in many gun systems, the detailed mechanism appears to be chemical rather than physical in nature. If this mechanism were understood, then measures to suppress the flash could be taken into account early in the design stages of a new weapon or weapon subsystem. This procedure would lead to substantial cost saving over the current practice of treating each case empirically after the fact.

Earlier<sup>1</sup> we discussed the problems that surround a popular suppression network that consists of two reactions. Recent work<sup>2</sup> has shown how complex such a network can be. In this paper we shall build upon this work and, in a systematic fashion, construct an advanced suppression network that forms a working hypothesis against which future experiments, both in the field and in the laboratory, can be tested.

---

1. J. M. Heimerl, "Muzzle Flash Suppression and Alkali Salt Inhibition," JANNAF 13th Plume Technology Meeting, Houston, TX, Vol I, pp. 413-418, 27-29 April 1982. Also available as: J. M. Heimerl, "Muzzle Flash and Alkali Salt Inhibition from an Elementary Kinetic Point of View," Technical Report ARBRL-TR-02479, March, 1983. AD A126 129.

2. A. J. Hynes, M. Steinberg and K. Schofield, "The Chemical Kinetics and Thermodynamics of Sodium Species in Oxygen-Rich Hydrogen Flames," J. Chem. Phys., Vol.80, pp. 2585-2597, 1984.

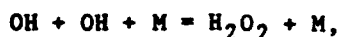


## II. THE CONSTRUCTION OF THE SUPPRESSION NETWORK

As with any new reaction network, three things must be determined: the reaction species, the network of reactions, and the rate coefficients for these reactions.

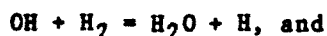
### A. THE SPECIES

The species that correspond to hydrogen as a fuel are: H, O, OH, H<sub>2</sub>, O<sub>2</sub>, HO<sub>2</sub>, and H<sub>2</sub>O. To include carbon monoxide as a fuel, the species CO and CO<sub>2</sub> must be added to this list. Since we are dealing with air we need also consider N<sub>2</sub>. However, the temperatures are such that N<sub>2</sub> acts only as a diluent. The species H<sub>2</sub>O<sub>2</sub> is absent from the above list. The reason for this neglect is as follows. The major formation path for H<sub>2</sub>O<sub>2</sub> is given by the three-body reaction:



whose reaction rate coefficient is given<sup>3</sup> by:  $1.3 \times 10^{22} \times T^{-2} \text{ cm}^6/\text{mole}^2\text{-sec}$ . At one atmosphere and a temperature of 1500 K the effective two-body rate

coefficient for this reaction is about  $5 \times 10^{10} \text{ cm}^3/\text{mole-sec}$ . Two-body reactions involving the OH radical have much greater values for their rate coefficients at 1500 K. For example, the reactions:



have values of about  $2 \times 10^{13}$ ,  $1 \times 10^{12}$  and  $6 \times 10^{12} \text{ cm}^3/\text{mole-sec}$ , respectively.<sup>3</sup> Thus, the species H<sub>2</sub>O<sub>2</sub> is not considered because at high temperatures its formation rate is much too small compared to other reactions involving OH.

There remains the selection of the suppressant species. The species Na, NaO, NaO<sub>2</sub> and NaOH were required<sup>2</sup> to describe adequately the inhibition of oxygen-rich hydrogen flames by sodium salt. By analogy we consider the corresponding potassium molecules: K, KO, KO<sub>2</sub> and KOH. In addition, since the muzzle effluent is fuel-rich we also consider the species KH.

Thus we shall consider 14 reactive species and the diluent N<sub>2</sub>.

---

3. J. Warnatz, "Survey of Rate Coefficients in the C/H/O System," Sandia Report SAND83-8606, February 1983.



Table 1 shows the list of 14 active species, their standard enthalpies of formation, and their absolute entropies (both at 298 K). These values are taken from standard sources, except for the enthalpy of  $\text{KO}_2$ , which is estimated in the appendix. Conversion to SI units can be made through the relation 4.184 joules = 1 calorie.

TABLE 1. LIST OF ACTIVE SPECIES

		enthalpy (kcal/mole)	entropy (cal/mole/K)	reference
1	H	52.10	27.40	a (p. 106)
2	K	21.30	38.30	b
3	O	59.60	38.50	a (p. 132)
4	$\text{H}_2$	0.00	31.20	b
5	KH	26.30	47.30	c, b
6	KO	17.50	56.90	c, b
7	OH	9.50	43.90	d
8	$\text{O}_2$	0.00	49.00	b
9	$\text{HO}_2$	3.50	54.40	e, b
10	$\text{H}_2\text{O}$	-57.80	45.10	b
11	KOH	-54.50	56.90	c, b
12	$\text{KO}_2$	-25.00	62.00	f
13	CO	-26.40	47.20	b
14	$\text{CO}_2$	-94.10	51.10	b

- a) J. Phys. & Chem. Ref. Data, Vol.4, 1975.  
 b) JANAF Thermochemical Tables, Second Edition, 1971.  
 c) J. Chem. Thermo., Vol.14, pp.1103-1113, 1982.  
 d) J. Phys. & Chem. Ref. Data, Vol.3, p.443, 1974.  
 e) J. Phys. Chem., Vol.87, pp.3479-3482, 1983.  
 f) This work, see appendix.

#### B. THE REACTION NETWORK

The next step in this process is the construction of a complete reaction network. We consider reactions involving as many as three molecules; i.e., we neglect reactions with four or more collision partners. We want to be sure that we have considered them all since the neglect of one implicitly assumes that its rate coefficient is zero. In principle, one simply writes down all combinations of the species to form the reactions. However, doing this manually for more than two or three species proves to be tedious and subject to error. Therefore, following Indritz, Maday and Sheinson,<sup>4</sup> we have constructed a computer program to perform the necessary bookkeeping operations to assure that all two- and three-body reactions are in fact considered. Since the forward and reverse directions of an elementary reaction are

4. D. Indritz, M. Maday and R. Sheinson, "Construction of Large Reaction Mechanisms," NRL Report 8498, October 1981.

automatically taken into account and since the reverse of three-body reactions of the form  $A + B + M \rightleftharpoons AB + M$  are unimolecular reactions, we automatically obtain the unimolecular decomposition reactions.

Table 2 shows the list of all exothermic two-body reactions that can be made from the species listed in Table 1. In order to avoid duplication, only those reactions that are exothermic at 298 K (i. e., have negative Gibbs free energies) are printed out. The selection of the Gibbs energy rather than the enthalpy of the reaction is arbitrary.

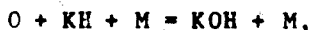
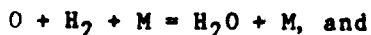
We can now begin the systematic elimination of the less important reactions. We make the reasonable assumption that if more than one bond is broken in a given reaction, it will have a very small rate coefficient and so can be neglected. With the exception of  $KO_2$ , the structures of all the species listed in Table 1 are known. We assume that the gas phase  $KO_2$

molecule has the same triangular geometry as the solid phase  $CaC_2$  molecule.<sup>5</sup> This assumption is consistent with our determination of the heat of formation of  $KO_2$ . (See appendix.)

We find that reactions 19, 22, 24-26, 30, 32-39, 47, 52 and 54 require more than one bond to be broken and so are deleted from the network. Note that reactions 25, 26, 34, 38, and 52 contain  $KO_2$  but require more than one bond to be broken no matter what the  $KO_2$  structure. On the other hand, reactions 8, 10, 49, and 55 do depend on the structure assumed for  $KO_2$ . With a triangular structure, these reactions require more than one bond to be broken and so they too are eliminated from the network.

As shown in Table 3, all reactions can conveniently be classified into: those reactions that are involved in the description of the hydrogen-oxygen flame, those reactions that describe the conversion of carbon monoxide to carbon dioxide, those reactions that are the potassium analogs of the sodium network of reference 2, those reactions that involve the species KH, and those reactions deleted (two categories).

Table 4 lists three-body reactions generated by the program. Not shown in this Table are the reactions:



because it is thought that the required rearrangement to form the product molecule is improbable. In addition, the four reactions:

---

5. For a discussion of the structure of these molecules in the solid phase, see for example, ADVANCED INORGANIC CHEMISTRY, A Comprehensive Text, by F. A. Cotton and G. Wilkinson, Wiley and Son, New York, fourth edition, p. 363 and p. 498, 1980.

TABLE 2. TWO-BODY REACTIONS

	<u>reaction</u>				<u>enthalpy</u>	<u>entropy</u>	<u>free energy</u>	
1	H	+ KH	= K	+ H <sub>2</sub>	-57.1000	-5.2000	-55.5504	1
2	H	+ KO	= K	+ OH	-38.8000	-2.1000	-38.1742	2
3	H	+ OH	= O	+ H <sub>2</sub>	-2.0000	-1.6000	-1.5232	3
4	H	+ HO <sub>2</sub>	= O	+ H <sub>2</sub> O	-53.8000	1.8000	-54.3364	4
5	H	+ HO <sub>2</sub>	= H <sub>2</sub>	+ O <sub>2</sub>	-55.6000	-1.6000	-55.1232	5
6	H	+ HO <sub>2</sub>	= OH	+ OH	-36.6000	6.0000	-38.3880	6
7	H	+ KOH	= K	+ H <sub>2</sub> O	-34.1000	-0.9000	-33.8318	7
8	H	+ KO <sub>2</sub>	= K	+ HO <sub>2</sub>	-2.3000	3.3000	-3.2834	8
9	H	+ KO <sub>2</sub>	= O	+ KOH	-22.0000	6.0000	-23.7880	9
10	H	+ KO <sub>2</sub>	= KH	+ O <sub>2</sub>	-0.8000	6.9000	-2.8562	10
11	H	+ KO <sub>2</sub>	= KO	+ OH	-0.1000	11.4000	-3.4972	11
12	K	+ HO <sub>2</sub>	= O	+ KOH	-19.7000	2.7000	-20.5046	12
13	K	+ HO <sub>2</sub>	= KO	+ OH	2.2000	8.1000	-0.2138	13
14	O	+ KH	= H	+ KO	-16.3000	-1.5000	-15.8530	14
15	O	+ KH	= K	+ OH	-55.1000	-3.6000	-54.0272	15
16	O	+ KO	= K	+ O <sub>2</sub>	-55.8000	-8.1000	-53.3862	16
17	O	+ OH	= H	+ O <sub>2</sub>	-17.0000	-6.0000	-15.2120	17
18	O	+ HO <sub>2</sub>	= OH	+ O <sub>2</sub>	-53.6000	0.0000	-53.6000	18
19	O	+ H <sub>2</sub> O	= H <sub>2</sub>	+ O <sub>2</sub>	-1.8000	-3.4000	-0.7868	19
20	O	+ KO <sub>2</sub>	= KO	+ O <sub>2</sub>	-17.1000	5.4000	-18.7092	20
21	H <sub>2</sub>	+ KO	= H	+ KOH	-19.9000	-3.8000	-18.7676	21
22	H <sub>2</sub>	+ KO	= K	+ H <sub>2</sub> O	-54.0000	-4.7000	-52.5994	22
23	H <sub>2</sub>	+ OH	= H	+ H <sub>2</sub> O	-15.2000	-2.6000	-14.4252	23
24	H <sub>2</sub>	+ HO <sub>2</sub>	= OH	+ H <sub>2</sub> O	-51.8000	3.4000	-52.8132	24
25	H <sub>2</sub>	+ KO <sub>2</sub>	= KO	+ H <sub>2</sub> O	-15.3000	8.8000	-17.9224	25
26	H <sub>2</sub>	+ KO <sub>2</sub>	= OH	+ KOH	-20.0000	7.6000	-22.2648	26
27	KH	+ KO	= K	+ KOH	-77.0000	-9.0000	-74.3180	27
28	KH	+ OH	= H	+ KOH	-38.2000	-6.9000	-36.1438	28
29	KH	+ OH	= K	+ H <sub>2</sub> O	-72.3000	-7.8000	-69.9756	29
30	KH	+ OH	= H <sub>2</sub>	+ KO	-18.3000	-3.1000	-17.3762	30
31	KH	+ O <sub>2</sub>	= K	+ HO <sub>2</sub>	-1.5000	-3.6000	-0.4272	31
32	KH	+ O <sub>2</sub>	= O	+ KOH	-21.2000	-0.9000	-20.9318	32
33	KH	+ O <sub>2</sub>	= KO	+ OH	0.7000	4.5000	-0.6410	33
34	KH	+ HO <sub>2</sub>	= H <sub>2</sub>	+ KO <sub>2</sub>	-54.8000	-8.5000	-52.2670	34
35	KH	+ HO <sub>2</sub>	= KO	+ H <sub>2</sub> O	-70.1000	0.3000	-70.1894	35
36	KH	+ HO <sub>2</sub>	= OH	+ KOH	-74.8000	-0.9000	-74.5318	36
37	KH	+ H <sub>2</sub> O	= H <sub>2</sub>	+ KOH	-23.0000	-4.3000	-21.7186	37
38	KH	+ KO <sub>2</sub>	= KO	+ KOH	-38.3000	4.5000	-39.6410	38
39	KH	+ CO <sub>2</sub>	= KOH	+ CO	-13.1000	5.7000	-14.7986	39
40	KO	+ KO	= K	+ KO <sub>2</sub>	-38.7000	-13.5000	-34.6770	40
41	KO	+ OH	= O	+ KOH	-21.9000	-5.4000	-20.2908	41
42	KO	+ HO <sub>2</sub>	= OH	+ KO <sub>2</sub>	-36.5000	-5.4000	-34.8908	42
43	KO	+ HO <sub>2</sub>	= O <sub>2</sub>	+ KOH	-75.5000	-5.4000	-73.8908	43
44	KO	+ H <sub>2</sub> O	= OH	+ KOH	-4.7000	-1.2000	-4.3424	44
45	KO	+ CO	= K	+ CO <sub>2</sub>	-63.9000	-14.7000	-59.5194	45
46	OH	+ OH	= O	+ H <sub>2</sub> O	-17.2000	-4.2000	-15.9484	46
47	OH	+ OH	= H <sub>2</sub>	+ O <sub>2</sub>	-19.0000	-7.6000	-16.7352	47

TABLE 2. TWO-BODY REACTIONS (continued)

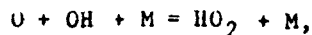
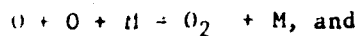
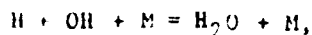
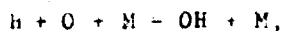
	<u>reaction</u>				<u>enthalpy</u>	<u>entropy</u>	<u>free energy</u>	
48	OH	+	HO <sub>2</sub>	= O <sub>2</sub> + H <sub>2</sub> O	-70.8000	-4.2000	-69.5484	48
49	OH	+	KO <sub>2</sub>	= O <sub>2</sub> + KOH	-39.0000	0.0000	-39.0000	49
50	OH	+	CO	= H + CO <sub>2</sub>	-25.1000	-12.6000	-21.3452	50
51	O <sub>2</sub>	+	CO	= O + CO <sub>2</sub>	-8.1000	-6.6000	-6.1332	51
52	HO <sub>2</sub>	+	KOH	= H <sub>2</sub> O + KO <sub>2</sub>	-31.8000	-4.2000	-30.5484	52
53	HO <sub>2</sub>	+	CO	= OH + CO <sub>2</sub>	-61.7000	-6.6000	-59.7332	53
54	H <sub>2</sub> O	+	CO	= H <sub>2</sub> + CO <sub>2</sub>	-9.9000	-10.0000	-6.9200	54
55	KO <sub>2</sub>	+	CO	= KO + CO <sub>2</sub>	-25.2000	-1.2000	-24.8424	55

TABLE 3. CATEGORIES OF REACTIONS

<u>classification</u>	<u>reaction numbers</u>
H <sub>2</sub> /O <sub>2</sub>	3-6, 17-18, 23, 46, 48
CO/CO <sub>2</sub>	45, 50-51, 53
K analogs to Na scheme	2, 7, 9, 11-13, 16, 20-21, 40-44
reactions involving KH	1, 14-15, 27-29, 31
deleted - multiple bond breaking	19, 22, 24-26, 30, 32-39, 47, 52, 54
deleted - depends on KO <sub>2</sub> structure	8, 10, 49, 55

TABLE 4. THREE-BODY REACTIONS

H	+	$\begin{Bmatrix} \text{H} \\ \text{K} \\ \text{KO} \\ \text{O}_2 \end{Bmatrix}$	+	M	=	$\begin{Bmatrix} \text{H}_2 \\ \text{KH} \\ \text{KOH} \\ \text{HO}_2 \end{Bmatrix}$	+	M
K	+	$\begin{Bmatrix} \text{O} \\ \text{OH} \\ \text{O}_2 \end{Bmatrix}$	+	M	=	$\begin{Bmatrix} \text{KO} \\ \text{KOH} \\ \text{KO}_2 \end{Bmatrix}$	+	M
O	+	$\begin{Bmatrix} \text{KO} \\ \text{CO} \end{Bmatrix}$	+	M	=	$\begin{Bmatrix} \text{KO}_2 \\ \text{CO}_2 \end{Bmatrix}$	+	M



do not appear because competing two-body reactions involving these radicals are known to be more important.

### C. THE RATE COEFFICIENTS

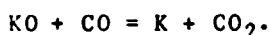
There are several compilations and evaluations of rate coefficients for the hydrogen-oxygen network,<sup>3,6,7</sup> and we have elected to use the most recent recommendations of Warnatz.<sup>3</sup>

He points out that reaction 4 of Table 2:

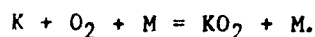


has been postulated, even though there is no direct evidence of its occurrence. In addition, he argues that indirect determinations show its rate coefficient to be small relative to the other two branches of the  $H + HO_2$  reaction (reactions 5 and 6 of Table 2). We accept his arguments and so do not consider this reaction further.

Warnatz<sup>3</sup> has also reviewed the values for the  $CO/CO_2$  rate coefficients and we have again used his recommendations. The one reaction of the  $CO/CO_2$  group not reviewed in the literature is:



Fortunately, it is known that the sodium analog of this reaction is fast<sup>8</sup> and so we assume a value of  $1 \times 10^{14} \text{ cm}^3/\text{mole-sec}$  for its rate coefficient. We use the published values of the rate coefficients for the sodium network<sup>2</sup> as those values appropriate to the potassium analog reactions. (See Table 3.) The single exception to this strategy is the value of the rate coefficient for the reaction:



6. G. Dixon-Lewis, "Kinetic Mechanism, Structure and Properties of Premixed Flames in Hydrogen-Oxygen-Nitrogen Mixtures," Proc. Roy. Soc. London, Vol.292, pp.45-99, 1979.

7. N. Cohen and K. R. Westberg, "Chemical Kinetic Data Sheets for High Temperature Chemical Reactions," J. Phys. Chem. Ref. Data, Vol.12, pp. 531-566, 1983.

8. J. Silver, Aerodyne Research Inc., private communication, 1984.

Here we have adopted Husain and Plane's<sup>9</sup> value for the corresponding sodium reaction,  $3 \times 10^{17} \text{ cm}^3/\text{mole-sec}$ , independent of temperature.

Those two-body rate coefficients for which we could find no published values were set at  $1 \times 10^{14} \text{ cm}^3/\text{mole-sec}$  ( $= 0.17 \times 10^{-09} \text{ cm}^3/\text{particle-sec}$ ). Similarly the three-body rate coefficients were assumed to have a rate coefficients that varied as  $A \times T^{-1}$ , where  $A = 10^{15} \text{ cm}^6/\text{mole}^2\text{-sec}$  ( $= 0.83 \times 10^{-30} \text{ cm}^3/\text{particle}^2\text{-sec}$ ). This network of 48 reactions and their respective rate coefficient parameters is shown in Table 5.

### III. RESULTS AND DISCUSSION

At this point, the network of reactions shown in Table 5 is ready for testing. The MEFF muzzle-flash-prediction code<sup>10</sup> is the only operational flash prediction code with detailed chemistry, it has been compared with other available codes and, to some extent, with observations,<sup>11</sup> and a user guide has been written to facilitate its use.<sup>12</sup> Reference 11 documents calculations made with MEFF using an earlier, less comprehensive 25-reaction network. We found that, in a nominal 155-mm howitzer simulation with a nominal M203 propelling charge, 1%  $\text{K}_2\text{SO}_4$  suppressant permitted flash, but 2.7%  $\text{K}_2\text{SO}_4$  suppressant suppressed the flash. Similarly, in an 81-mm mortar simulation, a nominal M10 propellant lacking suppressant flashed, but the addition of 2%  $\text{K}_2\text{SO}_4$  suppressed the flash, in agreement with observations.

We repeated the howitzer and mortar calculations with the 48-reaction network of Table 5, and the predictions of the MEFF flash-prediction code were nearly identical.

There still remained the question of whether or not the network of 48 reactions was a minimum needed to describe flash suppression. With the goal now of finding out whether the size of this reaction network could be further reduced, we took reactions 1-41 of Table 5 as the reaction network to describe the inhibition of a hydrogen-air flame. We employed our steady-state,

9. D. Husain and J. M. C. Plane, "Kinetic Investigation of the Reaction between  $\text{Na} + \text{O}_2 + \text{M}$  by Time-Resolved Atomic Resonance Absorption Spectroscopy," J. Chem. Soc. Faraday Trans. 2, Vol.78, pp. 163-178, 1982.

10. V. Yousefian, "Muzzle Flash Onset," Contractor Report ARBRL-CR-00477, February, 1982. AD B063 573L.

11. G. E. Keller, "An Evaluation of Muzzle Flash Prediction Models," U. S. Army Ballistic Research Laboratory ARBRL-MR-03318, November 1983.

12. G. E. Keller, "A MEFF User's Guide," U. S. Army Ballistic Research Laboratory ARBRL-MR-03362, July 1984.

TABLE 5. NETWORK OF ALL SINGLE-BOND-BREAKING REACTIONS

	<u>reaction</u>		<u>A</u>	<u>B</u>	<u>C</u>
1	OH	+ H <sub>2</sub> = H <sub>2</sub> O + H	0.17E-15	-1.6	-3298.8
2	H	+ O <sub>2</sub> = OH + O	0.20E-06	0.9	-16573.2
3	O	+ H <sub>2</sub> = OH + H	0.25E-16	-2.0	-7551.4
4	H	+ O <sub>2</sub> + M = HO <sub>2</sub> + M	0.55E-29	0.8	0.0
5	H	+ HO <sub>2</sub> = OH + OH	0.25E-09	0.0	-1003.5
6	H	+ HO <sub>2</sub> = H <sub>2</sub> + O <sub>2</sub>	0.42E-10	0.0	-693.5
7	OH	+ HO <sub>2</sub> = H <sub>2</sub> O + O <sub>2</sub>	0.33E-10	0.0	0.0
8	O	+ HO <sub>2</sub> = OH + O <sub>2</sub>	0.33E-10	0.0	0.0
9	H	+ H + M = H <sub>2</sub> + M	0.50E-29	1.0	0.0
10	H	+ H + H <sub>2</sub> = H <sub>2</sub> + H <sub>2</sub>	0.27E-30	0.6	0.0
11	OH	+ OH = O + H <sub>2</sub> O	0.25E-14	-1.1	0.0
12	H	+ KO <sub>2</sub> = KO + OH	0.12E-09	0.0	0.0
13	KO	+ H <sub>2</sub> O = OH + KOH	0.17E-09	0.0	0.0
14	H	+ KOH = K + H <sub>2</sub> O	0.17E-10	0.0	0.0
15	H	+ KO = K + OH	0.33E-10	0.0	0.0
16	H	+ KO <sub>2</sub> = O + KOH	0.33E-11	0.0	0.0
17	H	+ KO <sub>2</sub> = K + HO <sub>2</sub>	0.33E-10	0.0	0.0
18	K	+ HO <sub>2</sub> = O + KOH	0.66E-13	0.0	0.0
19	K	+ HO <sub>2</sub> = KO + OH	0.33E-11	0.0	0.0
20	O	+ KO = K + O <sub>2</sub>	0.33E-11	0.0	0.0
21	O	+ KO <sub>2</sub> = KO + O <sub>2</sub>	0.17E-11	0.0	0.0
22	H <sub>2</sub>	+ KO = H + KOH	0.83E-09	0.0	0.0
23	KO	+ OH = O + KOH	0.10E-09	0.0	0.0
24	KO	+ HO <sub>2</sub> = OH + KO <sub>2</sub>	0.33E-11	0.0	0.0
25	KO	+ HO <sub>2</sub> = O <sub>2</sub> + KOH	0.17E-09	0.0	0.0
26	OH	+ KO <sub>2</sub> = O <sub>2</sub> + KOH	0.50E-12	0.0	0.0
27	K	+ OH + M = KOH + M	0.25E-30	1.0	0.0
28	K	+ O <sub>2</sub> + M = KO <sub>2</sub> + M	0.83E-30	0.0	0.0
29	KO	+ KO = K + KO <sub>2</sub>	0.17E-09	0.0	0.0
30	H	+ KO + M = KOH + M	0.83E-30	1.0	0.0
31	O	+ KO + M = KO <sub>2</sub> + M	0.83E-30	1.0	0.0
32	K	+ O + M = KO + M	0.83E-30	1.0	0.0
33	H	+ KH = K + H <sub>2</sub>	0.17E-09	0.0	0.0
34	O	+ KH = H + KO	0.83E-10	0.0	0.0
35	O	+ KH = K + OH	0.83E-10	0.0	0.0
36	KH	+ KO = K + KOH	0.17E-09	0.0	0.0
37	KH	+ OH = H + KOH	0.17E-10	0.0	0.0
38	KH	+ OH = K + H <sub>2</sub> O	0.17E-09	0.0	0.0
39	KH	+ O <sub>2</sub> = K + HO <sub>2</sub>	0.17E-09	0.0	0.0
40	H	+ KO <sub>2</sub> = KH + O <sub>2</sub>	0.17E-09	0.0	0.0
41	H	+ K + M = KH + M	0.83E-30	1.0	0.0
42	CO	+ OH = H + CO <sub>2</sub>	0.73E-17	-1.5	741.0
43	CO	+ O <sub>2</sub> = O + CO <sub>2</sub>	0.42E-11	0.0	-47800.0
44	CO	+ HO <sub>2</sub> = OH + CO <sub>2</sub>	0.25E-09	0.0	-23590.0
45	CO <sub>2</sub>	+ O = CO + O <sub>2</sub>	0.28E-10	0.0	-52580.0
46	CO <sub>2</sub>	+ H = CO + OH	0.27E-09	0.0	-26300.0
47	O	+ CO + M = CO <sub>2</sub> + M	0.15E-33	0.0	4540.0
48	KO	+ CO = K + CO <sub>2</sub>	0.17E-09	0.0	0.0

The rate coefficient =  $A \times T^{-B} \times e^{C/RT}$   
 where A in units of cm-particle-sec  
 C in units of calorie/mole

laminar. flat-flame model<sup>13,14</sup> as a tool to make these decisions. The selection of input parameters other than the reactions and their rate coefficients will now be outlined.

The transport and thermodynamic parameters are shown in Table 6. The first line identifies the species and the five transport parameters. The first is the mass of the species, the second and third are the Lennard-Jones collision diameter (in Angstroms) and the Lennard-Jones potential well depth (in Kelvins), respectively, the fourth number is the dipole moment (in Debyes, where one Debye =  $10^{-18}$  cm<sup>3/2</sup> erg<sup>1/2</sup>), and the fifth number is the polarizability (in cubic Angstroms). These data were taken from Kee, et al.,<sup>15</sup> except for the potassium-containing molecules. The transport parameters for K, KOH and KO were assumed to be like those of their sodium analogs. The transport parameters for KO<sub>2</sub> were assumed to be like those of O<sub>3</sub>, while those of KH were assumed to be like argon. For each species there then follow the 14 thermodynamic parameters for use in the polynomial fits of Gordon and McBride.<sup>16</sup> These parameters are tabulated for all species we consider except KO<sub>2</sub>. The derivation of the KO<sub>2</sub> parameters is discussed in the appendix. The use of these parameters is detailed elsewhere.<sup>14</sup>

Next, we limited our study to the H<sub>2</sub>/air flame. The choice of fuel/oxidizer ratios was somewhat arbitrary except that we wanted to encompass a reasonably broad range. Figure 1, taken from reference 17, shows the flame velocity of H<sub>2</sub>/air mixtures vs. H<sub>2</sub> mole fraction. A mole fraction of 0.25 for H<sub>2</sub> gives a lean mixture while one of 0.50 gives a rich one. The flame velocities as read from this figure are 182.5 cm/sec and 287.5 cm/sec, respectively. In general, a given value of the flame velocity corresponds to two values of the mole fraction and we simply took the other two H<sub>2</sub> mole fractions for our test cases. This procedure gave us values of the equivalence ratio ranging from 0.79 to 3.88, as can be seen in Table 7.

This table shows the mole fraction initial conditions for the fuel, H<sub>2</sub>, the oxidizer, O<sub>2</sub>, the diluent, N<sub>2</sub>, and the inhibitor/suppressant, expressed as KOH. It also shows the computed flame speeds, S(cm/s), and the adiabatic flame temperature, T(Kelvin).

13. J. M. Heimerl and T. P. Coffee, "The Detailed Modeling of Premixed, Laminar Steady-State Flames. I. Ozone," Combustion and Flame, Vol.39, pp.301-315, 1980.

14. T. P. Coffee and J. M. Heimerl, "Transport Algorithms for Premixed, Laminar Steady-State Flames," Combustion and Flame, Vol.43, pp.273-289, 1981.

15. R. J. Kee, J. Warnatz and J. A. Miller, "A FORTRAN Computer Code Package for the Evaluation of Gas-Phase Viscosities, Conductivities, and Diffusion Coefficients," Sandia Report SAND83-8209, March 1983.

16. S. Gordon and B. J. McBride, "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouguet Detonations," NASA-SP-273, 1971. (1982 program version.)

17. J. Warnatz, "Calculation of the Structure of Laminar Flat Flames II: Flame Velocity and Structure of Freely Propagating Hydrogen-Oxygen and Hydrogen-Air Flames," Ber. Bunsenges. Phys. Chem., Vol.82, pp.643-649, 1978.



TABLE 6. TRANSPORT AND THERMODYNAMIC PARAMETERS

H	1.	2.05	145.	0.	0.					
.25000000D+01	0.		0.	0.		0.				H
.25474390D+05	-.45989841D+00		.25000000D+01	0.		0.				H
0.	0.		.25474390D+05	-.45989841D+00						H
OH	17.	2.75	80.	0.	0.					
.28897814D+01	.10005879D-02		-.22048807D-06	.20191288D-10		-.39409831D-15				OH
.38857042D+04	.55566427D+01		.38737300D+01	-.13393772D-02		.16348351D-05				OH
-.52133639D-09	.41826974D-13		.35802348D+04	.34202406D+00						OH
O	16.	2.75	80.	0.	0.					
.25342961D+01	-.12478170D-04		-.12562724D-07	.69029862D-11		-.63797095D-15				O
.29231108D+05	.49628591D+01		.30309401D+01	-.22525853D-02		.39824540D-05				O
-.32604921D-08	.10152035D-11		.29136526D+05	.26099342D+01						O
HO <sub>2</sub>	33.	3.46	107.	0.	1.6					
.40173060D+01	.22172883D-02		-.57710171D-06	.71372882D-10		-.36458591D-14				HO <sub>2</sub>
-.11412445D+04	.37846051D+01		.35964102D+01	.52500748D-03		.75118344D-05				HO <sub>2</sub>
-.95674952D-08	.36597628D-11		-.89333502D+03	.66372671D+01						HO <sub>2</sub>
H <sub>2</sub>	2.	2.92	38.	0.	.79					
.30558123D+01	.59740400D-03		-.16747471D-08	-.21247544D-10		.25195487D-14				H <sub>2</sub>
-.86168476D+03	-.17207073D+01		.29432327D+01	.34815509D-02		-.77713819D-05				H <sub>2</sub>
.74997496D-08	-.25203379D-11		-.97695413D+03	-.18186137D+01						H <sub>2</sub>
O <sub>2</sub>	32.	3.372	128.7	0.	1.6					
.36122139D+01	.74853166D-03		-.19820647D-06	.33749008D-10		-.23907374D-14				O <sub>2</sub>
-.11978151D+04	.36703307D+01		.37837135D+01	-.30233634D-02		.99492751D-05				O <sub>2</sub>
-.98189101D-08	.33031825D-11		-.10638107D+04	.36416345D+01						O <sub>2</sub>
H <sub>2</sub> O	18.	2.6	572.	1.844	0.					
.27167633D+01	.29451374D-02		-.80224374D-06	.10226682D-09		-.48472145D-14				H <sub>2</sub> O
-.29905826D+05	.66305671D+01		.40701275D+01	-.11084499D-02		.41521180D-05				H <sub>2</sub> O
-.29637404D-08	.80702103D-12		-.30279722D+05	-.32270046D+00						H <sub>2</sub> O
N <sub>2</sub>	28.	3.62	97.	0.	1.76					
.28532899D+01	.16022128D-02		-.62936893D-06	.11441022D-09		-.78057465D-14				N <sub>2</sub>
-.89008093D+03	.63964897D+01		.37044177D+01	-.14218753D-02		.28670392D-05				N <sub>2</sub>
-.12028885D-08	-.13954677D-13		-.10640795D+04	.22336285D+01						N <sub>2</sub>
KO <sub>2</sub>	71.	4.69	39.4	0.	0.					
0.56193353D+01	0.15509417D-02		0.68222055D-06	0.13299869D-09		0.95542863D-14				
-0.14355891D+05	-0.17198447D+01		0.34337129D+01	0.67246085D-02		-0.33216077D-05				
-0.16047227D-08	0.13795100D-11		0.13720689D+05	0.97559016D+01		FIGGER, ANDREWS				
K	39.	3.567	1375.	0.	0.					LIKE Na
0.25673650D+01	-0.14933596D-03		0.12342444D-06	-0.53394240D-10		0.11948426D-13				
0.99550531D+04	0.46642081D+01		0.24930967D+01	0.50164177D-04		-0.12751224D-06				
0.13540491D-09	-0.51145936D-13		0.99786360D+04	0.50560438D+01		TRANDATA2				

TABLE 6. TRANSPORT AND THERMODYNAMIC PARAMETERS(continued)

KOH	56.	3.804	1962.	0.	0.	LIKE NaOH
0.56400949D+01	0.12510226D-02	-0.34984547D-06	0.44566993D-10	-0.20870279D-14		
-0.29698732D+05	-0.40568187D+01	0.40733441D+01	0.97217945D-02	-0.15988804D-04		
0.12148353D-07	-0.33709342D-11	-0.29506558D+05	0.29222373D+01		TRANDATA2	
KO	55.	3.812	383.	0.	0.	LIKE NaO
0.44244778D+01	0.19936155D-03	-0.37128837D-07	0.71308300D-11	-0.50369687D-15		
0.72052331D+04	0.32945055D+01	0.37410778D+01	0.31242017D-02	-0.48020039D-05		
0.34660605D-08	-0.93599791D-12	0.73368714D+04	0.65537609D+01		TRANDATA2	
KH	40.	3.542	93.3	0.	0.	LIKE Ar
0.39603386D+01	0.72190323D-03	-0.26918715D-06	0.52617300D-10	-0.37872683D-14		
0.13501837D+05	0.84218060D+00	0.28157756D+01	0.39871060D-02	-0.33410548D-05		
0.88602942D-09	0.11402847D-12	0.13805838D+05	0.67120145D+01		TRANDATA2	

TABLE 7. INITIAL CONDITIONS FOR AND SELECTED OUTPUT FROM THE STEADY-STATE, LAMINAR, FLAT-FLAME MODEL

equivalence ratio	INITIAL CONDITIONS				OUTPUT	
	XH <sub>2</sub>	XO <sub>2</sub>	XN <sub>2</sub>	XKOH	S	T
0.79	.25000	.15750	.59250	.0	174.6	2168
	.24950	.15740	.59210	.001	182.3	2164
	.24875	.15671	.58954	.005	152.1	2153
1.28	.35000	.13650	.51350	.0	285.4	2338
	.34965	.13636	.51299	.001	315.6	2334
	.34825	.13582	.51093	.005	335.7	2320
	.34650	.13514	.50836	.01	296.9	2302
	.34300	.13377	.50323	.02	192.6	2267
2.38	.50000	.10500	.39500	.0	275.1	1938
	.50000	.10500	.39426	.00074	297.9	1937
	.49750	.10448	.39302	.005	280.2	1920
	.49500	.10395	.39105	.01	132.6	1902
3.88	.62000	.07980	.30020	.0	177.0	1581
	.61938	.07972	.29990	.001	177.6	1577
	.61876	.07964	.29960	.002	131.0	1574

An analysis (a so-called screening analysis) of each of these flames showed that several other reactions could be eliminated. These reactions were found to contribute less than 1% to the formation or destruction of any species over the computational space. The results of these eliminations is the 32-reaction network which is shown in Table 8. (The reactions retain the numbering of Table 5.)

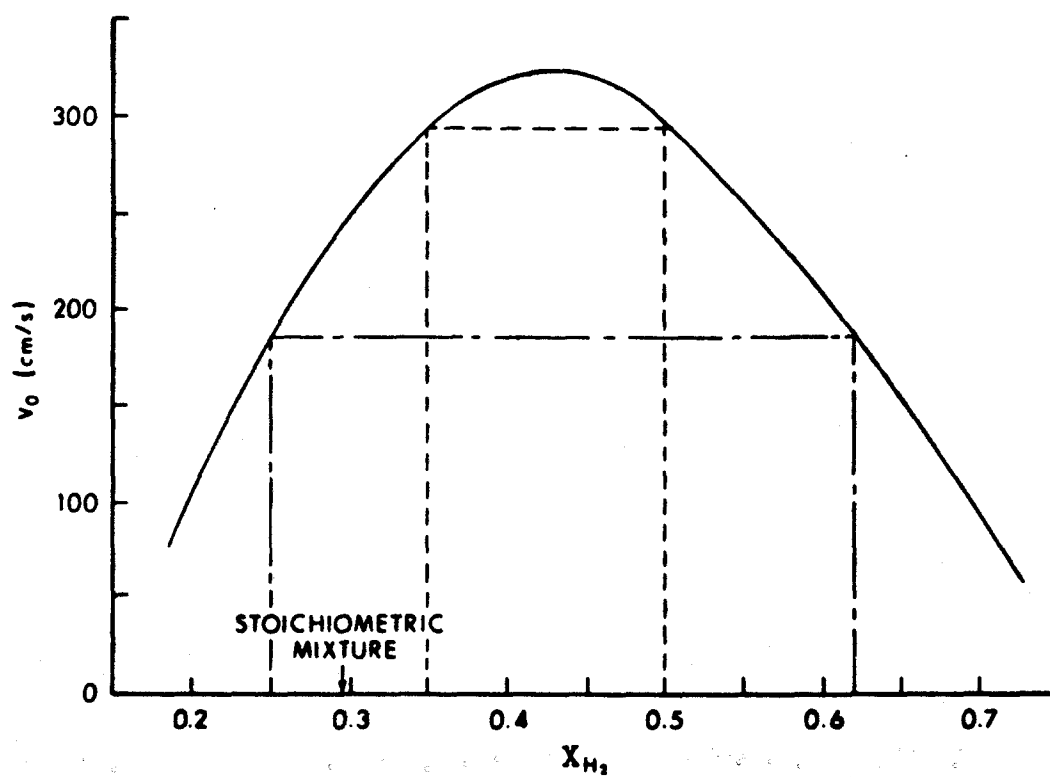


Figure 1. Flame Velocity in the  $H_2$ /Air Flame as a Function of  $H_2$  Mole Fraction

TABLE 8. ABBREVIATED REACTION NETWORK

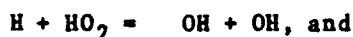
<u>reaction</u>				<u>A</u>	<u>B</u>	<u>C</u>
1	OH	+ H <sub>2</sub>	= H <sub>2</sub> O + H	0.17E-15	-1.6	-3298.8
2	H	+ O <sub>2</sub>	= OH + O	0.20E-06	0.9	-16573.2
3	O	+ H <sub>2</sub>	= OH + H	0.25E-16	-2.0	-7551.4
4	H	+ O <sub>2</sub> + M	= HO <sub>2</sub> + M	0.55E-29	0.8	0.0
5	H	+ HO <sub>2</sub>	= OH + OH	0.25E-09	0.0	-1003.5
6	H	+ HO <sub>2</sub>	= H <sub>2</sub> + O <sub>2</sub>	0.42E-10	0.0	-693.5
7	OH	+ HO <sub>2</sub>	= H <sub>2</sub> O + O <sub>2</sub>	0.33E-10	0.0	0.0
8	O	+ HO <sub>2</sub>	= OH + O <sub>2</sub>	0.33E-10	0.0	0.0
9	H	+ H + M	= H <sub>2</sub> + M	0.50E-29	1.0	0.0
10	H	+ H + H <sub>2</sub>	= H <sub>2</sub> + H <sub>2</sub>	0.27E-30	0.6	0.0
11	OH	+ OH	= O + H <sub>2</sub> O	0.25E-14	-1.1	0.0
12	H	+ KO <sub>2</sub>	= KO + OH	0.12E-09	0.0	0.0
13	KO	+ H <sub>2</sub> O	= OH + KOH	0.17E-09	0.0	0.0
14	H	+ KOH	= K + H <sub>2</sub> O	0.17E-10	0.0	0.0
16	H	+ KO <sub>2</sub>	= O + KOH	0.33E-11	0.0	0.0
17	H	+ KO <sub>2</sub>	= K + HO <sub>2</sub>	0.33E-10	0.0	0.0
19	K	+ HO <sub>2</sub>	= KO + OH	0.33E-11	0.0	0.0
21	O	+ KO <sub>2</sub>	= KO + O <sub>2</sub>	0.17E-11	0.0	0.0
22	H <sub>2</sub>	+ KO	= H + KOH	0.83E-09	0.0	0.0
28	K	+ O <sub>2</sub> + M	= KO <sub>2</sub> + M	0.83E-30	0.0	0.0
29	KO	+ KO	= K + KO <sub>2</sub>	0.17E-09	0.0	0.0
33	H	+ KH	= K + H <sub>2</sub>	0.17E-09	0.0	0.0
38	KH	+ OH	= K + H <sub>2</sub> O	0.17E-09	0.0	0.0
39	KH	+ O <sub>2</sub>	= K + HO <sub>2</sub>	0.17E-09	0.0	0.0
40	H	+ KO <sub>2</sub>	= KH + O <sub>2</sub>	0.17E-09	0.0	0.0
42	CO	+ OH	= H + CO <sub>2</sub>	0.73E-17	-1.5	741.0
43	CO	+ O <sub>2</sub>	= O + CO <sub>2</sub>	0.42E-11	0.0	-47800.0
44	CO	+ HO <sub>2</sub>	= OH + CO <sub>2</sub>	0.25E-09	0.0	-23590.0
45	CO <sub>2</sub>	+ O	= CO + O <sub>2</sub>	0.28E-10	0.0	-52580.0
46	CO <sub>2</sub>	+ H	= CO + OH	0.27E-09	0.0	-26300.0
47	O	+ CO + M	= CO <sub>2</sub> + M	0.15E-33	0.0	4540.0
48	KO	+ CO	= K + CO <sub>2</sub>	0.17E-09	0.0	0.0

The rate coefficient =  $A \times T^B \times e^{C/RT}$   
 where A in units of cm-particle-sec  
 C in units of calorie/mole

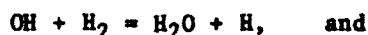
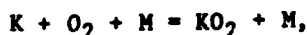
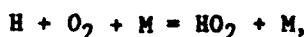
This 32-reaction network was also used as input for the MEFF code computations and results similar to the 48 reaction network were obtained. In addition, both hydrogen-air subsets of Tables 5 and 8, when used as input to the flat-flame code, yielded nearly identical species, temperature, and heat release profiles. We conclude that the abbreviated reaction network of Table 8 constitutes a minimal descriptive suppression network.

Caution must be urged at this point. If the values of any of the assumed rate coefficients, upon measurement, prove to be significantly less than given in Table 8, then, because of the non-linear couplings among all of the species and between the species and the temperature, the entire network given in Table 5 should be reexamined.

Referring to Table 7, one can see that the computed flame velocity drops with continued addition of suppressant, while the temperature is hardly affected. This is not surprising since we are dealing with a series of different flames and there need not be any simple correlation among them. To see this most easily, consider the two flames with initial fuel and oxidizer values of 0.50000 and 0.10500, respectively (equivalence ratio = 2.38). The only difference lies in the trace amount of KOH added at the expense of the diluent N<sub>2</sub>. The adiabatic flame temperature changes by one degree but the computed flame speed shows a noticeable change. Analysis shows that near the peaks of the respective heat release functions, the elementary chemistry has altered radically. In the case of no KOH addition, the rate of increase of temperature is governed by the reactions:



and by diffusion processes. In the case of the small addition of KOH, the rate of increase of temperature is governed by:



all listed in rank order.

The above points out the importance of obtaining reliable values for key reactions such as  $K + O_2 + M = KO_2 + M$ . Were we to repeat any of these computations we would use the most recent measurements of Husain and Plane<sup>18</sup> and of Silver et al.<sup>19</sup> Their values for this potassium reaction show that our assumed value is low by a factor ranging from 5 at 300 K to 50% at 3000 K. Had we used this value somewhat more, KO<sub>2</sub> would have been formed; however, this should not qualitatively affect our results.

The fact that the rate coefficient for the reaction forming KO<sub>2</sub> is so great has implications for the experimentalist. When we first began to use the flat-flame code we initialized all of the potassium as the atomic species, K. Analysis showed that within the space scale we were using (about 0.01 cm),

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18. D. Husain and J. M. C. Plane, "Kinetic Investigation of the Reaction between  $K + O_2 + M$  by Time-Resolved Atomic Resonance Absorption Spectroscopy," J. Chem. Soc. Faraday Trans. 2, Vol.78, pp.1175-1194, 1982.

19. J. A. Silver, M. S. Zahniser, A. C. Stanton, and C. E. Kolb, "Temperature Dependent Termolecular Reaction Rate Constants For Potassium and Sodium Superoxide Formation," Aerodyne Report ARI-RR 381, January 1984. See also: paper #68 Twentieth Symposium (International) on Combustion, the University of Michigan, Ann Arbor Michigan, 12-17 Aug 1984.

all the K was converted to  $KO_2$  at the cold (298 K) boundary. The conclusion we draw is that unless special precautions are taken, the addition of free atomic potassium to an input gas stream containing  $O_2$  would result in the conversion of the K to  $KO_2$  before the gases could reach the burner surface. (In the execution of the flat-flame computer code this difficulty was easily overcome by assigning all the initial potassium to the species KOH.)

Table 8 shows that the species KH is involved in only a few reactions. Analysis shows that the KH is almost exclusively formed by the reaction:



The computed concentration of  $KO_2$  can be large for an intermediate species and in our computed results it is probably too low. To be able to tell whether or not the species KH will actually play a significant role in the flash suppression network will require a measurement of this reaction rate coefficient.

#### IV. SUMMARY

An advanced suppression network has been constructed by extending the inhibition network of Hynes et al.<sup>2</sup> First, the most likely species to be involved in flash suppression were considered. These species include: K, KO,  $KO_2$ , KOH, and KH. From these species a complete set of 55 two-body and 15 three-body reactions was constructed. Standard chemical kinetic arguments were used to reduce the number of reactions to 48. Use of screening analysis upon the output of flat-flame code computations enabled the network to be further reduced to 32 reactions. Both the extended set of 48 reactions and the abbreviated set of 32 reactions gave nearly identical results when used as the reaction network for the MEFF muzzle-flash-prediction code, for both howitzer and mortar calculations. In addition, when used as input for the flat-flame code, the respective hydrogen-air subsets, with and without potassium, also yielded the same computed profiles for the species, temperature, and heat release. Further analysis showed that  $KO_2$  is mainly formed from  $K + O_2 + M = KO_2 + M$  and that KH is mainly formed from  $H + KO_2 = KH + O_2$ . The former is currently under investigation<sup>19</sup> while the latter is a candidate for future work.

#### ACKNOWLEDGEMENTS

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APPENDIX A  
APPROXIMATE PROPERTIES OF THE  $\text{KO}_2$  MOLECULE



## APPENDIX A

### Approximate Properties Of The $\text{KO}_2$ Molecule

The one-dimensional, laminar, flat-flame code we used demands species-dependent thermodynamic functions of temperature. This was accomplished by using the polynomial expressions of Gordon and McBride.<sup>A-1</sup> For each reaction species, the specific heat, enthalpy, and entropy as functions of temperature are given in the form:

$$C_p/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4,$$

$$H_T/RT = a_1 + a_2T/2 + a_3T^2/3 + a_4T^3/4 + a_5T^4/5 + a_6/T,$$

and

$$S_T/R = a_1 \ln T + a_2T + a_3T^2/2 + a_4T^3/3 + a_5T^4/4 + a_7.$$

Parameters corresponding to each species considered in this report are documented except for the species  $\text{KO}_2$ . Suitable parameters for  $\text{KO}_2$  can be generated provided that the heat of formation, moments of inertia, and the normal mode frequencies are known. First consider an estimation of the  $\text{KO}_2$  heat of formation.

Figger, Schrepp, and Zhu<sup>A-2</sup> used spectroscopic techniques to determine a lower limit for the K- $\text{O}_2$  bond energy of  $(45.2 \pm 2.4)\text{kcal/mole}$ . It is our present task then to relate this bond energy to the heat (enthalpy) of formation.

The standard enthalpy of formation of any compound is the net heat of reaction by which it is formed from its elements, the reactants and products all being in a given standard state. A convenient standard state for a substance is the state in which it is stable at 298.15K and one atmosphere pressure. By convention the enthalpies of the chemical elements in this particular state are set equal to zero.

Using the first law of thermodynamics and considering only PV work, we find the change in enthalpy can be written as:

$$\Delta H = \Delta U + \Delta(PV).$$

By  $\Delta(PV)$  we mean the change in PV for the entire system; that is, the PV of the products minus the PV of the reactants for the particular chemical reaction. For reactions in the gas phase, the values of  $\Delta(PV)$  depend on the change in the number of moles of gas as a result of the reaction under consideration. From the ideal gas equation we can write:

$$\Delta(PV) = RT\Delta n.$$

A-1. S. Gordon and B. J. McBride, "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouguet Detonations," NASA-SP-273, 1971. (1982 program version.)

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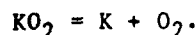


Thus:

$$\Delta H = \Delta U + RT\Delta n,$$

where by  $\Delta n$  we mean the number of moles of gaseous products minus the number of moles of gaseous reactants.

For the present case:



We note that at zero degrees absolute:

$$\Delta H_o = \Delta U_o = \Delta H_r.$$

Now:

$$\Delta H_r = \Delta H_{fo}(K) + \Delta H_{fo}(O_2) - \Delta H_{fo}(KO_2)$$

and substituting values from Table A-1 we find

$$45.2 = 21.5 + 0.0 - \Delta H_{fo}(KO_2)$$

or

$$\Delta H_{fo}(KO_2) = -23.7 \text{ kcal/mole.}$$

TABLE A-1. SELECTED THERMODYNAMIC VALUES

Species	$\Delta H_{fo}$	$\Delta H_{f298}$	+/-	$(H_o - H_{298})$	Reference
K	21.522	21.31	0.20	-1.481	A-8
O <sub>2</sub>	0.0	0.0		-2.075	A-8
O <sub>3</sub>	34.8	34.2	0.4	-2.474	A-8
H <sub>2</sub> O	-57.103	-57.7979		-2.367	A-8
KOH	-54.6	-55.6	3.0	-2.730	*

KO<sub>2</sub> (bond energy) = (45.2 +/- 2.4) kcal/mole A-2

\* J. Chem. Phys. Ref. Data, Vol.3, p.432, 1974.

To find the heat of formation at 298.15K we recognize that for the reaction above where the stoichiometric coefficients are unity:

$$\Delta H_{fT} = \Delta H_{f298} + (H_T - H_{298})_{\text{compound}} - \text{SUM}(H_T - H_{298}),$$

where the sum is taken over the elements in their standard state. For this case we have:

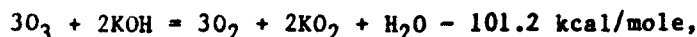
$$\Delta H_{fo}(KO_2) = \Delta H_{f298}(KO_2) + (H_o - H_{298})_{KO_2} - (H_o - H_{298})_K - (H_o - H_{298})_{O_2}.$$

Substituting appropriate values from Table A-1 we find:

$$\Delta H_{f298}(KO_2) = -(25 \pm 3) \text{ kcal/mole},$$

where we have approximated the difference in enthalpy for  $KO_2$  by that for  $O_3$ .

As a check on this value we note that the room temperature heat of reaction for:



was reported by the Vol'nov et al.<sup>A-3</sup> Using the values given in Table A-1, we find:

$$\Delta H_{f298}(KO_2) = -(26 \pm 3) \text{ kcal/mole},$$

in good agreement with our above estimate.

Both Raman spectra<sup>A-4</sup> and electron spin resonance spectra<sup>A-5</sup> of  $KO_2$  in rare gas matrices show that the structure is that of an isosceles triangle. Since the actual structure of the gas phase molecule has not been determined, we assume that the gas phase molecule also has an isosceles triangle structure, identical with that of the solid. Andrews<sup>A-6</sup> estimated the K-O distance in  $KO_2$  to be 2.28 Å, while Kassatichkin and Kotow<sup>A-7</sup> obtained  $(1.28 \pm 0.07)$  Å as the distance between adjacent oxygen atoms. With these data the moments of inertia can be computed. They are: 2.18, 14.0, and 16.18 in units of  $10^{-39} \text{ gm-cm}^2$ .

The last data we require for the  $KO_2$  molecule are the values of the normal mode frequencies. Smardzewski and Andrews<sup>A-4</sup> measured the fundamental frequency to be  $1108 \text{ cm}^{-1}$ . They also measured the symmetric interionic stretching mode frequency of  $307.5 \text{ cm}^{-1}$ . Based on analogy with ozone<sup>A-8</sup> we estimate the antisymmetric normal vibration frequency to be  $1100 \text{ cm}^{-1}$ .

A-3. I. I. Vol'nov, V. N. Chamova, and E. I. Latysheva, "Mechanism of Alkali Metal Ozonide Formation," Izv. Akad. Nauk. SSSR, Ser. Khim., pp.1183-1187, 1967. As quoted in Chem.Abs., Vol.68, p.6291, 1968.

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A-7. W. Kassatichkin and W. Kotow, "Structure of Potassium Tetroxide," J. Chem. Phys., Vol.4, p.458, 1936.

A-8. JANAF Thermochemical Tables, 2nd Ed., D. R. Stull and H. Prophet, NSRDS-NBS-73, June 1971.

Noting that the assumed geometry for  $\text{KO}_2$  yields a symmetry number of two, we have all the required input information to generate the Gordon and McBride coefficients.<sup>A-9</sup> The values for the  $a_i$  are shown in Table A-2.

TABLE A-2. GORDON AND MCBRIDE COEFFICIENTS,  $a_i$ , FOR  $\text{KO}_2$

<u>i</u>	<u>T&gt;1000K</u>	<u>T&lt;1000K</u>
1	.56193353E+01	.34337129E+01
2	.15509417E-02	.67246035E-02
3	-.68222055E-06	-.33216077E-05
4	.13299869E-09	-.16047227E-08
5	-.95542863E-14	.13795100E-11
6	-.14355891E+05	-.13720689E+05
7	-.17198447E+01	.97559016E+01

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Use of these  $a_i$  and  $R=1.9872$  cal/mole/K yields a room temperature value for the entropy of  $\text{KO}_2$  of 62 cal/mole/K.

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A-9. B. J. McBride and S. Gordon, "FORTRAN IV Program for Calculation of Thermodynamic Data," NASA TN D-4097, 1967.

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